

on the theory of supersolidity

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We present a microscopic, many-body argument for supersolidity. We also illustrate the origin of rotons in a Bose system.

In physics the most fascinating phenomena are perhaps so-called macroscopic quantum phenomena, such as superfluidity, partially due to that they are anti-intuitive at a visible scale. It might look unlikely to get a clear theoretical picture of these phenomena since that quantum many-body problems are complex problems. However, some direct analysis still can be performed and some understanding can be obtained at the very fundamental level, for example, the construction of Laughlin's wavefunction for fractional quantum Hall effect. In this paper, we attempt to argue that supersolidity [1] is a natural consequence of Bose exchange symmetry through a direct analysis of the many-body wave functions of a Bose system, our analysis also reveals the origin of rotons in a Bose system, which is another fascinating issue in condensed matter physics.

The knowledge of superfluidity has accumulated through the efforts of several generations of physicists [2]. Landau [3] first related superfluidity with the properties of the spectrum of a system, specifically, the quasi-particle spectrum. Bloch's [4] and Leggett's [5] works clearly point out that a more transparent way to understand this phenomenon is based on the properties of many-body dispersion spectrum, i.e., the lowest eigen energies of the system at given momenta. When there exist local minima in the dispersion spectrum, the energy barriers which separate the minima will prevent the decay of current carried by the states corresponding the minima (see Fig. 2 for example), thus superfluidity occurs [8].

We have argued in [6] that the existence of the local minima in the dispersion spectrum of a Bose system could be understood in terms of Bose exchange symmetry. Let us consider a 2D periodic Bose system with N particle, with a finite-range repulsive interaction and with a square geometry (see Fig. 1), The Hamiltonian takes a form

$$H = - \sum_{i=1}^N \frac{\hbar^2}{2MR^2} \frac{\partial^2}{\partial \theta_i^2} + g \sum_{i < j}^N f(\theta_i - \theta_j), \quad (1)$$

Where M is the mass of a particle, g is the interaction strength, f describes the form of a repulsive interaction, $2\pi R$ is the linear size of the system. $\theta_i = (x_i, y_i)/R$ where (x_i, y_i) are the coordinates of the i -th particle. We

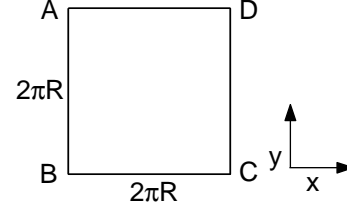


Figure 1: The geometry of a 2D periodic system. The edge AB is identified with DC and BC identified with AD . The linear size of the system is $2\pi R$.

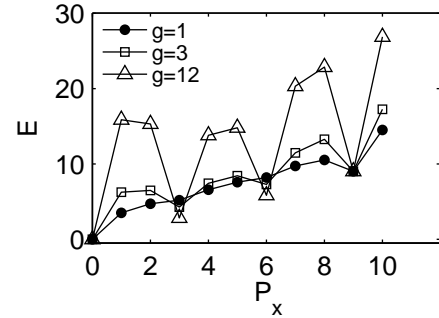


Figure 2: The spectra of yrast states with $P_y = 0$, relative to the ground state energy, for three systems with $N = 9$, and having various interaction strengths g . the interaction takes a form of $f(\theta) = 4\pi^2 e^{-\theta^2/4\xi^2} / (4\pi\xi^2)$ with $\xi = 2\pi/15$.

will adopt the unit system generated by \hbar , R and M , except that the energy is in the unit of $\hbar^2/2MR^2$ where a factor of a half is involved for convenience.

The many-body spectrum can be labeled by the momentum of the system $\mathbf{P} = (P_x, P_y)$, since P_x, P_y are good quantum numbers due to the translational symmetry. We consider part of the spectrum, $E = E(P_x, P_y)$, where E is the minimum energy at the given (P_x, P_y) . We will call the many-body states corresponding this dispersion spectrum the yrast states, following convention in nuclear physics.

Due to Galileo invariance [4, 6], we can derive the full yrast spectrum if part of this spectrum in the regime $0 \leq P_x \leq N$, $0 \leq P_y \leq N$ is known. Particularly, we can derive all local minima of the spectrum and realize that there is an upper momentum limit beyond which no supercurrents exist any more, i.e., there exists a critical

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velocity [4, 6]. We will only focus on the structure of the yrast spectrum in the momentum regime $0 \leq P_x \leq N$, $0 \leq P_y \leq N$ in the rest of this paper.

The perturbation analysis of the yrast states and dispersion spectrum of the system at small g , is straightforward and presented in [6]. For example, the yrast states for $0 \leq P_x \leq N$, $P_y = 0$ are approximated well by Fock states $|(0,0)^N(1,0)^0\rangle, |(0,0)^{N-1}(1,0)^1\rangle, |(0,0)^{N-2}(1,0)^2\rangle, \dots, |(0,0)^0(1,0)^N\rangle$, where (m,n) , a pair of integers, denotes the single particle orbit $\psi_{m,n}(x,y) = 1/(2\pi)e^{imx/R+iny/R}$ and $|(0,0)^{j_1}(1,0)^{j_2}\rangle$ denotes a Fock state with j_1 particles occupying orbits $(0,0)$ and j_2 particles in orbits $(1,0)$. These Fock states will have the same (direct) Fock energy while the exchange energy, as a function of P_x , has a parabolic behavior, $E_{ex} \propto g(N - P_x)P_x$. This behavior of the exchange energy, without any classical analog, is responsible for the possible existence of local minimum of the dispersion spectrum at $(P_x, P_y) = (N, 0)$. In [6], we also present the second micromany-body argument for the exchange origin of superfluidity. By comparing the dispersion spectrum of a spinless Bose system and that of a corresponding spinor Bose system, one can naturally imagine that the possible energy barriers separating two neighboring minima of dispersion spectrum (of a spinless system) will become more apparent with increasing g , i.e., strong interaction enhances superfluidity.

In this paper, we will present another many-body argument for the quantum origin of superfluidity, which illustrate in a direct way the role of exchange symmetry in determining the dispersion spectrum of the systems. This argument also indicate a natural compatibility of superfluidity and crystalline ordering, on the contrast to previous common beliefs that crystalline ordering will destroy superfluidity. Supersolidity is a natural consequence of this compatibility.

We consider the system specified above with $N = 9$, the generalization for $N = m^2$, where m is an integer [7], is straightforward. The dispersion spectra shows that with large g there are also supercurrents at $(P_x, P_y) = (3, 0), (6, 0)$ besides the one at $(P_x, P_y) = (9, 0)$ (see Fig. 2). The supercurrent states at $\mathbf{P} = (3, 0)$ and $(6, 0)$ are rather surprising, in which it is impossible that all nine particles occupy the same orbits. This 'new' supercurrents can be explained.

A many-body state of the system can be written in the spatial presentation

$$|\psi\rangle = \sum_{x_1, x_2, \dots, x_9} \psi(x_1, x_2, \dots, x_9) |x_1, x_2, \dots, x_9\rangle \quad (2)$$

one might refer to each state $|x_1, x_2, \dots, x_9\rangle$ as a configuration with the first particle at position x_1 , the second at x_2 , ..., the ninth at x_9 .

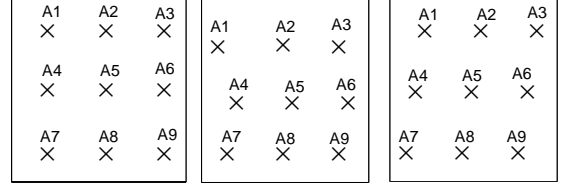


Figure 3: Some examples of configurations with $2\pi/3 - x -$ symmetry and with rather small interaction energies. Crosses mark the positions denoted by A_i s.

and the interaction energy of the state has the form of,

$$E_{int}^\psi = \langle \psi | g \sum_{i < j}^N f(x_i - x_j) | \psi \rangle \quad (3)$$

$$= \sum_{x_1, \dots, x_9} |\psi(x_1, \dots, x_9)|^2 g \left(\sum_{i < j}^N f(x_i - x_j) \right) \quad (4)$$

which can be interpreted as average of the interaction energy of each configuration, with weight being the square module of the wavefunction. The configurations with small interaction energy shall be largely explored by the yrast states at large g , in which the interaction energy dominates the kinetic energy.

We shall consider a group of configurations with a certain discrete translational symmetry and its relationship with yrast states. The symmetry is following. If one configuration is translated by a mount of $2\pi/3R$ along x axis, the first particles will be in the previous position of the second particle ($x_1 \rightarrow x_2$), the second particles will reach the previous position of the third particle ($x_2 \rightarrow x_3$), and $x_3 \rightarrow x_1$, $x_4 \rightarrow x_5 \rightarrow x_6 \rightarrow x_4$, $x_7 \rightarrow x_8 \rightarrow x_9 \rightarrow x_7$. We label the positions of nine particles of this configuration by A_1, A_2, \dots, A_9 , i.e., $x_1 = A_1, x_2 = A_2, \dots, x_9 = A_9$. Thus after the translation, $x_1 = A_2, x_2 = A_3, x_3 = A_1, \dots, x_9 = A_7$.

We refer to this symmetry as $2\pi/3 - x -$ symmetry. Obviously, most configurations with $2\pi/3 - x -$ symmetry has a relatively small interaction energy since the particles are well separated along x axis, (see Fig. 3 for examples).

We shall argue that the configurations with $2\pi/3 - x -$ symmetry can only be accommodated (with a non-zero weight) by yrast states at $P_x = 0, 3, 6, 9, \dots$.

First, with this translation, the wavefunction associated with the configurations changes to be,

$$\begin{aligned} \Psi(x_1 = A_2, \dots, x_9 = A_7) &\equiv \psi(A_1 + b, \dots, A_9 + b) \\ &= e^{ib\hat{P}/\hbar} \psi(A_1, A_2, \dots, A_9) \end{aligned} \quad (5)$$

Where $b = (2\pi/3R, 0)$, $\hat{P} = (\hat{P}_x, \hat{P}_y)$ is the momentum operator. For eigenstates of the \hat{P} , $b\hat{P}/\hbar = P_x/3 * 2\pi$ with P_x in the unit we specified above.

Due to Bose exchange symmetry, the wavefunction is invariant under any permutation of the coordinates of particles, thus

$$\psi(A_2, A_3, \dots, A_7) = \psi(A_1, A_2, \dots, A_9). \quad (6)$$

Combining Eqs. 5, 6, one is led to

$$(e^{i\frac{2\pi}{3}P_x} - 1)\psi(A_1, A_2, A_3; A_4, A_5, A_6; A_7, A_8, A_9) = 0. \quad (7)$$

Thus $\psi(A_1, A_2, A_3, A_4, A_5, A_6, A_7, A_8, A_9) = 0$ at $P_x \neq 0, 3, 6, \dots$. The configurations with $2\pi/3 - x$ -symmetry can't be effectively involved in those yrast states with $P_x \neq 0, 3, 6, \dots$.

One can also note that if one configuration is not involved in a yrast state $|\psi\rangle$, its neighboring configurations can't be effectively involved in $|\psi\rangle$. For a configuration with first particle at position B_1 , the second particle in position B_2, \dots , in its neighboring configurations, the first particle is at position $B_1 + \delta_1$ where δ_1 is small position shift, and the second particle is at $B_2 + \delta_2$ with δ_2 being small, \dots . If $\psi(B_1, B_2, \dots, B_9) = 0$, then $|\psi(B_1 + \delta_1, B_2 + \delta_2, \dots, B_9 + \delta_9)|$ can't be large, otherwise the value of the wavefunction changes dramatically from $(x_1, x_2, \dots) = (B_1, B_2, \dots)$, to $(x_1, x_2, \dots) = (B_1 + \delta_1, B_2 + \delta_2, \dots)$, which means that the wavefunction has a large gradient and thus a large kinetic energy (density) near this neighboring configuration, but large kinetic energy (density) shall be avoided in the yrast states which pursue the minimum energy at given momenta.

Therefore, the yrast states at $P_x = 0, 3, 6, 9, \dots$ can use the configurations with $2\pi/3 - x$ -symmetry and their neighboring configurations to lower their interaction energy while the yrast states at other P_x can not. Similarly, the yrast states at $P_y = 0, 3, 6, 9, \dots$ can effectively access configurations with $2\pi/3 - y$ -symmetry and their neighboring configurations to lower the interaction energy while the states at other P_y can not. At sufficient large g , the yrast states at $(P_x, P_y) = (3, 0), (6, 0), (9, 0), (3, 3), \dots$, will become supercurrent states, with energies lower than the energies of their neighboring yrast states.

The configurations with $2\pi/3 - x, y$ -symmetry are also the fundamental components to build an inner crystal-like structure in the system, one thus draw a conclusion that only those yrast states with particular momentum values can support such inner crystal-like structures, they are supercurrent states. The inner crystal-like structure of the ground state at large g can be seen clearly in the plot of pair correlation function (see Fig. 4), which is defined as

$$\rho(\theta, \theta_A) = \frac{\langle \psi | \sum_{i \neq j} \delta(\theta - \theta_i) \delta(\theta_A - \theta_j) | \psi \rangle}{\langle \psi | \sum_j \delta(\theta_A - \theta_j) | \psi \rangle} \quad (8)$$

where θ_A is the referees point.

The above discussions can be generalized to systems with large N and to 3D systems straightforwardly. In a 2D system with square periodic boundary geometry, with $N = m^2$ [7], and with large g , the yrast spectrum

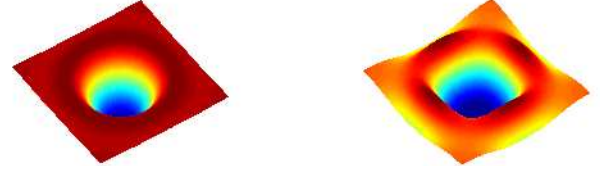


Figure 4: Pair correlation profile of the ground state of a system with $g = 1$ (left) and of a system with $g = 12$ (right). The reference point θ_A is located at the center. $N = 9$. At rather small g , $g = 1$, the system has short-range correlations but no long-range correlations and is in a gas-like or liquid-like phase (left). At large g , $g = 12$, the system has long-range correlations and is in a solid-like phase (right).

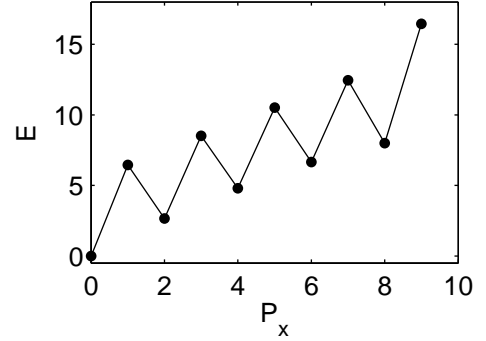


Figure 5: The yrast spectrum of a 3D periodic system, relative to the ground state energy. $P_y = P_z = 0$. $N = 8$. the interaction is $V(\theta) = (2\pi)^3 g e^{-\theta^2/4\xi^2} / (\sqrt{4\pi}\xi)^3$, with $g = 6$, $\xi = 3\pi/20$, where $\theta = (\theta_x, \theta_y, \theta_z)$ is the difference between the generalized angular coordinates of two interacting particles.

will have local minima at $(P_x, P_y) = (m, 0), (2m, 0), \dots, (m, m), (2m, m), \dots, (m, m)$, due to the compatibility of the yrast states at these momenta with the particle configurations with $2\pi/m - x, y$ -symmetry. In a 3D system with cubic periodic boundary geometry and with $N = m^3$, the yrast states at $(P_x, P_y, P_z) = (m, 0, 0), (2m, 0, 0), \dots, (m, m, 0), (2m, m, 0), \dots, (m, m, m), \dots, (m^3, m^3, m^3)$ can become supercurrent states for their accommodations of the configurations with $2\pi/m - x, y, z$ -symmetry. Numerical results of a 3D periodic cubic system with $N = 8$ are plotted in Fig. 5.

The above argument for exchange origin of superfluidity can also be applied to a system with an interparticle interaction which is repulsive at short range and attractive at long range, for example, the Helium system. In these systems, the configurations with that type of discrete translation symmetries are still energetically favorable and the states compatible with these configurations can become supercurrent states. One might naturally speculate that supersolidity can be observed in neon systems, much like the case of helium systems [9].

It is interesting to note that the smallest momentum of a supercurrent in a Bose system with large repulsive in-

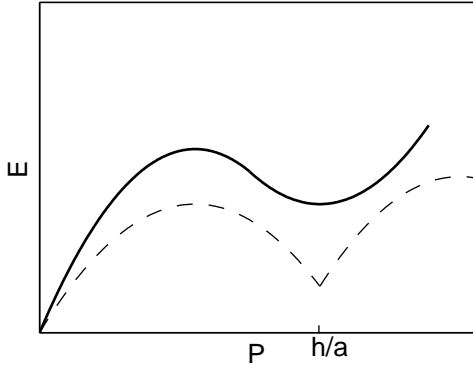


Figure 6: Schematic plots of the quasiparticle dispersion (solid line) and yrast spectrum (dashed line) of a repulsive Bose system. Quasiparticles generally do not exist beyond a threshold where certain decay channels become allowed [11]. h is Planck's constant.

interaction is $\delta p = N^{1/d}$ (d is the dimensionality) and that it corresponds to the inverse of the average particle distance a . In liquid ^4He , the momentum corresponding to rotons in quasiparticle spectrum is also around h/a (h is Planck's constant), which naturally suggests that rotons are due to the local minimum of the yrast spectrum. The quasiparticle dispersion curve lies above the many-body dispersion curve, as illustrated schematically in Fig. 6. Corresponding to the local minima of the yrast spectrum at momentum h/a , there are rotons in the quasiparticle spectrum.

In conclusion, we present a microscopic many-body argument for supersolidity. We also predict possible supersolidity in ^{20}Ne and in ^{22}Ne .

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 - [8] Here one ignores the probability for a supercurrent state, a yrast state corresponding to a local minimum, to decay into another supercurrent state (with a less energy). In such a decay process, the system emits a quantum with a certain energy and with a large momentum which is at least of the order of h/a where a is the average interparticle distance. Depending on its own low energy spectrum, the environment may not be capable of absorbing this quantum and thus this decay process is unlikely to occur.
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 - [10] In a $2D$ or $3D$ periodic Bose system, both the yrast spectrum and the quasiparticle dispersion are anisotropic. If one ignores the anisotropy of the quasiparticle dispersion and considers the average of the lowest quasiparticle energies at $P = |\mathbf{P}|$, then this average is expected to have a minimum around the momentum h/a .
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